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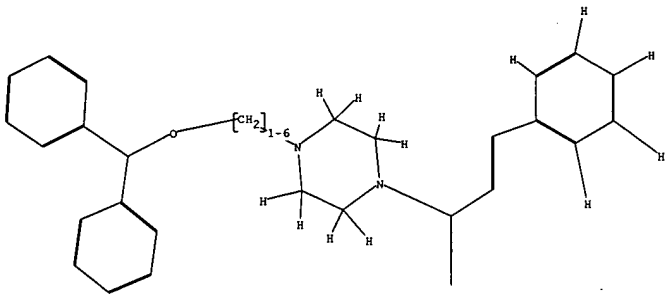
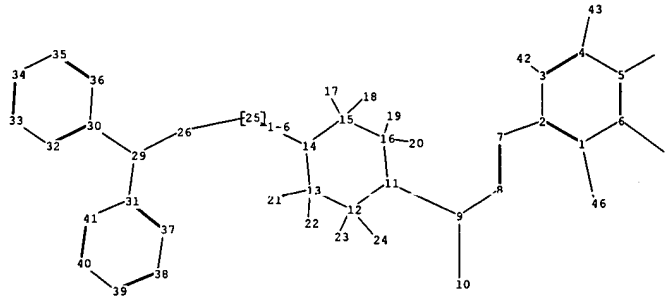




update 9/30/08

chain nodes :
7 8 9 17 18 19 20 21 22 23 24 25 26 29 42 43 44 45 46
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16 30 31 32 33 34 35 36 37 38 39 40 41
ring/chain nodes :
10
chain bonds :
1-46 2-7 3-42 4-43 5-44 6-45 7-8 8-9 9-10 9-11 12-23 12-24 13-21 13-22
14-25 15-17 15-18 16-19 16-20 25-26 26-29 29-30 29-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 30-32 30-36
31-37 31-41 32-33 33-34 34-35 35-36 37-38 38-39 39-40 40-41
exact/norm bonds :
9-11 11-12 11-16 12-13 13-14 14-15 15-16 26-29
exact bonds :
1-46 2-7 3-42 4-43 5-44 6-45 7-8 8-9 9-10 12-23 12-24 13-21 13-22 14-25
15-17 15-18 16-19 16-20 25-26 29-30 29-31
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 30-32 30-36 31-37 31-41 32-33 33-34 34-35 35-36
37-38 38-39 39-40 40-41

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 29:CLASS 30:Atom
31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
41:Atom 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS

=> S L1 FULL
FULL SEARCH INITIATED 22:19:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

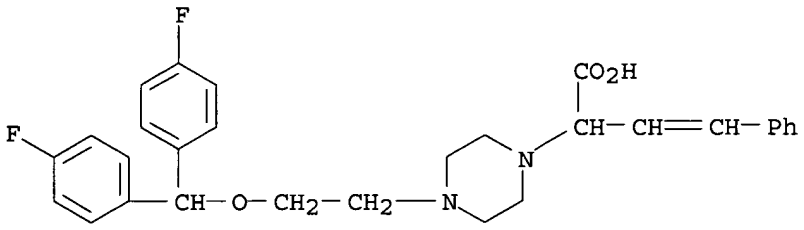
L3 2 SEA SSS FUL L1

=> D ALL

L3 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN 350583-56-1 REGISTRY
CN 1-Piperazineacetic acid,
4-[2-[bis(4-fluorophenyl)methoxy]ethyl]-.alpha.-(2-phenylethenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H30 F2 N2 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	3
C4N2	NC2NC2	6	C4N2	46.383.1	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	18.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	137	pH 4	(1) ACD
Bioconc. Factor (BCF)	160	pH 7	(1) ACD
Bioconc. Factor (BCF)	125	pH 8	(1) ACD
Bioconc. Factor (BCF)	8.85	pH 10	(1) ACD
Boiling Point (BP)	623.1+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	97.02+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	330.6+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	28.6	pH 1	(1) ACD
Koc (KOC)	218	pH 4	(1) ACD
Koc (KOC)	255	pH 7	(1) ACD
Koc (KOC)	200	pH 8	(1) ACD

Koc (KOC)	14.1	pH 10	(1) ACD
logD (LOGD)	3.05	pH 1	(1) ACD
logD (LOGD)	3.93	pH 4	(1) ACD
logD (LOGD)	4.00	pH 7	(1) ACD
logD (LOGD)	3.89	pH 8	(1) ACD
logD (LOGD)	2.74	pH 10	(1) ACD
logP (LOGP)	6.503+/-0.668		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	492.56		(1) ACD
pKa (PKA)	3.93+/-0.10	Most Acidic	(1) ACD
pKa (PKA)	8.47+/-0.50	Most Basic	(1) ACD
Vapor Pressure (VP)	2.19E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:107255 CA
TI Preparation of polypharmacophoric agents
IN Hanson, Robert N.; Babich, John W.
PA Biostream Therapeutics, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D241-04
ICS C07D211-34; C07D211-44; C07D223-26
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001051474	A2	20010719	WO 2001-US1035	20010111
	WO 2001051474	A3	20011206		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	US 2002042357	A1	20020411	US 2001-758957	20010111
	EP 1257541	A2	20021120	EP 2001-902026	20010111
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	JP 2003519689	T2	20030624	JP 2001-551856	20010111
PRAI	US 2000-175617P	20000111			
	WO 2001-US1035	20010111			

AB Title compds. (I) comprise a scaffold bearing .gtoreq.2 pharmacophore units selected from D1, D2, D3,
and D4 agonists, (ir)reversible monoamine inhibitors, monoamine transporter inhibitors, COMT inhibitors,
MAO inhibitors, and dopamine transporter inhibitors. I interact with .gtoreq.2 biol. targets. Thus,
(E)-PhZCH(CO2H)CH:CHPh (Z = piperidine-4,1-diyl) was prepd. Data for biol. activity of I were given.
ST polypharmacophoric agent prepn; dopaminergic system agent prepn
IT Dopamine agonists
(D1; prepn. of polypharmacophoric agents)
IT Dopamine agonists

(D2; prepn. of polypharmacophoric agents)
IT Dopamine agonists
(D3; prepn. of polypharmacophoric agents)
IT Nervous system
(Huntington's chorea, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(attention deficit disorder, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(autism, treatment; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(dopamine-transporting, inhibitors; prepn. of polypharmacophoric agents)
IT Nervous system
(dopaminergic; prepn. of polypharmacophoric agents)
IT Monoamines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(monoamine-transporting, inhibitors; prepn. of polypharmacophoric agents)
IT Anti-inflammatory agents
Antidepressants
Antiobesity agents
Pharmacophores
(prepn. of polypharmacophoric agents)
IT Alzheimer's disease
(treatment; prepn. of polypharmacophoric agents)
IT 9001-66-5, monoamine oxidase 9012-25-3, Catechol O-methyl transferase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT 67469-69-6P 350583-53-8P 350583-56-1P 350583-58-3P 350583-59-4P 350583-60-7P 350583-61-8P
350583-62-9P 350583-63-0P 350583-64-1P 350583-65-2P 350583-66-3P 350583-67-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of polypharmacophoric agents)

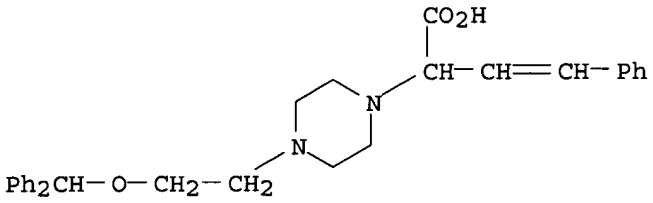
=> D ALL 2

L3 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN 350583-53-8 REGISTRY
CN 1-Piperazineacetic acid,
4-[2-(diphenylmethoxy)ethyl]-.alpha.-(2-phenylethenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H32 N2 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence

EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	3
C4N2	NC2NC2	6	C4N2	46.383.1	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	14.9	pH 1	(1) ACD
Bioconc. Factor (BCF)	112	pH 4	(1) ACD
Bioconc. Factor (BCF)	134	pH 7	(1) ACD
Bioconc. Factor (BCF)	105	pH 8	(1) ACD
Bioconc. Factor (BCF)	7.50	pH 10	(1) ACD
Boiling Point (BP)	621.5+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	96.80+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	329.6+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	24.9	pH 1	(1) ACD
Koc (KOC)	188	pH 4	(1) ACD
Koc (KOC)	224	pH 7	(1) ACD
Koc (KOC)	177	pH 8	(1) ACD
Koc (KOC)	12.6	pH 10	(1) ACD
logD (LOGD)	2.94	pH 1	(1) ACD
logD (LOGD)	3.82	pH 4	(1) ACD
logD (LOGD)	3.89	pH 7	(1) ACD
logD (LOGD)	3.79	pH 8	(1) ACD
logD (LOGD)	2.64	pH 10	(1) ACD
logP (LOGP)	6.400+/-0.547		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	456.58		(1) ACD
pKa (PKA)	3.93+/-0.10	Most Acidic	(1) ACD
pKa (PKA)	8.48+/-0.50	Most Basic	(1) ACD
Vapor Pressure (VP)	2.64E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:107255 CA

TI Preparation of polypharmacophoric agents
IN Hanson, Robert N.; Babich, John W.
PA Biostream Therapeutics, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D241-04
ICS C07D211-34; C07D211-44; C07D223-26
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001051474	A2	20010719	WO 2001-US1035	20010111
	WO 2001051474	A3	20011206		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	US 2002042357	A1	20020411	US 2001-758957	20010111
	EP 1257541	A2	20021120	EP 2001-902026	20010111
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	JP 2003519689	T2	20030624	JP 2001-551856	20010111
PRAI	US 2000-175617P	20000111			
	WO 2001-US1035	20010111			

AB Title compds. (I) comprise a scaffold bearing .gtoreq.2 pharmacophore units selected from D1, D2, D3,
and D4 agonists, (ir)reversible monoamine inhibitors, monoamine transporter inhibitors, COMT inhibitors,
MAO inhibitors, and dopamine transporter inhibitors. I interact with .gtoreq.2 biol. targets. Thus,
(E)-PhZCH(CO2H)CH:CHPh (Z = piperidine-4,1-diyl) was prepd. Data for biol. activity of I were given.

ST polypharmacophoric agent prepn; dopaminergic system agent prepn
IT Dopamine agonists
(D1; prepn. of polypharmacophoric agents)
IT Dopamine agonists
(D2; prepn. of polypharmacophoric agents)
IT Dopamine agonists
(D3; prepn. of polypharmacophoric agents)
IT Nervous system
(Huntington's chorea, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(attention deficit disorder, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(autism, treatment; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(dopamine-transporting, inhibitors; prepn. of polypharmacophoric agents)
IT Nervous system
(dopaminergic; prepn. of polypharmacophoric agents)
IT Monoamines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(monoamine-transporting, inhibitors; prepn. of polypharmacophoric agents)

IT Anti-inflammatory agents
Antidepressants
Antiobesity agents
Pharmacophores
(prepn. of polypharmacophoric agents)
IT Alzheimer's disease
(treatment; prepn. of polypharmacophoric agents)
IT 9001-66-5, monoamine oxidase 9012-25-3, Catechol O-methyl transferase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT 67469-69-6P 350583-53-8P 350583-56-1P 350583-58-3P 350583-59-4P 350583-60-7P 350583-61-8P
350583-62-9P 350583-63-0P 350583-64-1P 350583-65-2P 350583-66-3P 350583-67-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
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